Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the

application:

Listing of Claims

1. (Currently Amended):   A method for selecting at least one lead-candidate

compound capable of binding as a ligand to a protein from a database of trial compounds

comprising information on atomic types [[and]], covalent bonds and three-dimensional structures

of compounds in the database, comprising:

a) inputting at least one query molecule that is known to bind, or expected to be capable

of binding, to the protein;

b) screening lead-candidate compounds from the compound database by matching modes

of covalent bonds between the query molecule and the trial compounds stored in the database and

judging similarity of partial structures of the query molecule and the trial compounds based on

two-dimensional graphs of the query molecule and the trial compounds where each atom is

represented as a node and each covalent bond is represented as an arc; [[and]]

c) estimating a binding scheme of the lead-candidate compounds to the protein based on

three-dimensional information and binding scheme of the query molecule to the protein and

based on correspondence of the mode of covalent bonds of the partial structures of the query

molecule and the trial compounds; and

[[c)]]d) outputting at least one lead-candidate compound capable of binding to the protein

to a display, a user, a readily accessible memory, or other computer on a network.

2-5. (Canceled)

6. (Currently Amended) The method of claim 1, ~~wherein the compound database comprises information on three-dimensional structures of the trial compounds, and wherein step (b)~~ which further comprises:

~~estimating a binding scheme of the lead-candidate compounds to the protein based on three-dimensional information and binding scheme of the query molecule to the protein and based on correspondence of the partial structures of the query molecule and the trial compounds;~~

calculating one or more parameters relating to interaction between the lead-candidate compounds and the protein; and

screening the lead-candidate compounds capable of binding as a ligand to the protein based on the parameters relating to interaction between the lead-candidate compounds and the protein.

7. (Currently Amended): The method of claim 1, wherein ~~the compound database comprises information on three-dimensional structures of the trial compounds, and wherein the step (b) further comprises:~~

~~estimating~~ the protein is a virtual receptor model which represents physicochemical environment of the ligand binding site of the protein based on information of three-dimensional structures of one or more known ligands capable of binding to the protein[[;]]

~~fitting the lead-candidate compound to the virtual receptor model and judging goodness~~

of fit of the trial compounds to the virtual receptor model; and

screening the lead candidate compounds capable of binding as a ligand to the protein based on the goodness of fit.

8-10. (Canceled)

11. (Previously Presented) The method of claim 1, wherein step (a) further comprises constructing the structure of the at least one query molecule by an automatic structure construction method.

12. (Canceled)

13. (Canceled)

14. (New) The method of claim 7, further comprising screening the lead-candidate compounds capable of binding as a ligand to the protein based on the goodness of fit of the lead-candidate compounds to the virtual receptor model.